

**Machine Learning in Materials Processing &
Characterization**

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5 **Abstract**

6 This course provides students with essential skills and practical knowledge to
 7 harness machine learning techniques for accelerating materials discovery and de-
 8 sign. Specifically tailored for students interested in the new BSc program “KI-
 9 Materialtechnologie”/AI for materials technology”, it provides hands-on experience
 10 with core and advanced machine learning methods—including neural networks, opti-
 11 mization strategies, and generative modelling—to tackle real-world materials science
 12 problems. The course focuses on experimental data: microstructures, images, spec-
 13 tra, and processing parameters, connecting the messy, nonlinear world of processing
 14 and characterization signals with machine learning tools.

15 **Plain Language Summary**

16 This course teaches how to apply machine learning to materials science problems,
 17 focusing on experimental data from characterization techniques (microscopy, spec-
 18 troscopy) and processing parameters. Students learn to build ML pipelines for mi-
 19 crostructure classification, process prediction, and spectral analysis, with emphasis
 20 on understanding the physics of data formation and avoiding common pitfalls in
 21 experimental ML workflows.

22 **1 Machine Learning in Materials Processing & Characterization**

23 **4th Semester – 5 ECTS, 2h lecture + 2h exercises per week**

24 **1.1 Synergy Map**

- 25 • **This course:** What ML can do with experimental data: microstructures,
 26 images, spectra, processing parameters.
- 27 • **Parallel ML intro course:** Teaches generic ML algorithms and image pro-
 28 cessing foundations (skimage, Fourier, wavelets, SVMs, Bayes classifiers).
- 29 • **“Materials Genomics” course:** Focuses on materials databases, descrip-
 30 tors, crystal graph representations, DFT data, high-throughput workflows,
 31 surrogate models.

32 **1.2 Week-by-Week Curriculum (14 weeks)**

33 **1.2.1 Unit I — Foundations: From Materials Signals to Machine Learn-**
 34 **ing (Weeks 1–3)**

35 **1.2.1.1 Week 1 – What makes materials data special?**

- 36 • Types of data: micrographs, EBSD, EDS, EELS, XRD, process logs, thermal
 37 profiles, deformation curves.
- 38 • PSPP (Processing–Structure–Property–Performance) as a data graph.
- 39 • Why vision-based ML and time-series ML are central to processing & charac-
 40 terization.

41 **1.2.1.2 Week 2 – Image formation & the physics of data**

- 42 • How characterization creates data: resolution, contrast mechanisms, artifacts.
- 43 • Fourier optics intuition for students with their ML-intro foundations.
- 44 • Sampling, aliasing, denoising as model-based priors.

45 **1.2.1.3 Week 3 – Experimental data quality & ML-readiness**

- 46 • Annotation, segmentation, inter-annotator variance.
- 47 • Train/test leakage in materials workflows.

48 (*These first three weeks ensure students understand why ML behaves differently on*
 49 *materials data compared to CIFs and DFT databases in the other course.*)

50 **1.2.2 Unit II — ML for Microstructure: Vision & Representation**
51 (**Weeks 4–6**)

52 1.2.2.1 Week 4 – Classical microstructure quantification & its ML extension

- 53 • Grain size, phase fractions, orientation maps, lineal intercepts.
- 54 • From hand-crafted features → learned representations.

55 1.2.2.2 Week 5 – Convolutional Neural Networks for microstructure classification

- 56 • CNN filters as microstructure interpreters.
- 57 • Example tasks: grain-boundary segmentation, precipitate detection, melt pool
58 defects.

59 1.2.2.3 Week 6 – Transfer learning & data scarcity in materials characterization

- 60 • How to train a model with 200 images instead of 200k.
- 61 • Representations from ImageNet vs self-supervised pretraining on microstruc-
62 tures.

63 **1.2.3 Unit III — ML in Processing: Time-Series, Optimization, Ther-
64 mal/Mechanical Data (Weeks 7–9)**

65 1.2.3.1 Week 7 – Process monitoring & time-series ML

- 66 • Process logs: temperature cycles, additive manufacturing melt pool monitor-
67 ing, SPS, rolling, heat treatment.
- 68 • Hidden Markov models, ARIMA, random forest regressors, RNNs (light intro-
69 duction).

70 1.2.3.2 Week 8 – Process → structure regression & uncertainty

- 71 • Gaussian Processes (synergy with Materials Genomics' surrogate models, but
72 here linked to experimental data).
- 73 • Uncertainty as a tool for process design.

74 1.2.3.3 Week 9 – Inverse problems in processing

- 75 • ML-guided process maps (AM: laser power vs scan speed; metallurgy: TTT/CCT
76 approximations).
- 77 • Physics-informed ML vs naive regression.

78 (*This unit ensures profoundly processing-centered ML content—distinct from ge-
79 nomics's structure-first world.*)

80 **1.2.4 Unit IV — ML for Characterization Signals (Weeks 10–12)**

81 1.2.4.1 Week 10 – Spectral data: ML for XRD, EELS, EDS

- 82 • Peak detection, denoising, background removal.
- 83 • Dimensionality reduction (PCA, NMF, ICA).

84 1.2.4.2 Week 11 – ML for microscopy automation

- 85 • Auto-focusing, drift correction, parameter selection.
- 86 • Vision-based defect detection in EBSD or TEM.

87 1.2.4.3 Week 12 – Multi-modal data fusion

- 88 • Combining images + spectra + process parameters.
- 89 • Early vs late fusion.

90 (*This module draws synergy with your research—students love learning real lab-
91 relevant problems.*)

92 **1.2.5 Unit V — Project + Reflection (Weeks 13–14)**

93 1.2.5.1 Week 13 – Mini-project workshop

94 **Projects could be:**

- 95 • Predict microhardness from heat-treatment + microstructure images.

- 96 • Segment phases in SEM images.
97 • Detect porosity in AM melt pool images.
98 • Denoise EELS/XRD spectra.
99 • Build a process map using Gaussian Processes.

100 **Students must show:**

- 101 1. data prep → 2. model selection → 3. evaluation → 4. uncertainty → 5. interpretation.

103 *1.2.5.2 Week 14 – Presentations + critical evaluation*

- 104 • Focus on explainability (CAMs, SHAP for simple models).
105 • Reflect on why ML sometimes fails on materials data.
106 • Wrap-up: Where ML is genuinely changing materials characterization.

107 **1.3 Learning Outcomes**

108 Students completing this course should be able to:

- 109 • Interpret materials characterization and processing data in an ML-ready way.
110 • Build ML pipelines for microstructure classification, process prediction, and
111 spectral analysis.
112 • Understand the physics of image/signal formation well enough to avoid
113 “garbage in → garbage out”.
114 • Evaluate uncertainty and biases in experimental ML models.
115 • Combine processing and characterization data for property prediction.
116 • Critically evaluate claims about ML in materials science. ##

117 **1.4 Lab possibilities:**

- 118 • **Lab:** Exploring real microscopy datasets; noise, metadata, units.
119 • **Lab:** Fourier & wavelet inspection of SEM/TEM/optical micrographs.
120 • **Lab:** Correct vs broken experimental ML pipelines; data-leak horror stories.
121 • **Lab:** Using scikit-image to extract features; PCA on microstructure descrip-
122 tors.
123 • **Lab:** Fine-tuning a pretrained model on SEM/optical images.
124 • **Lab:** Predicting hardness from heat-treatment curves.
125 • **Lab:** GP on process parameters (e.g., cooling rate → microstructure metric).
126 • **Lab:** Building process maps using ML surrogate models.
127 • **Lab:** NMF decomposition of EELS datasets; automatic phase identification in
128 XRD.
129 • **Lab:** Implementing a simple “AI autofocus” or EBSD pattern classifier.
130 • **Lab:** Fusing XRD + microstructure representations for property prediction.

131 **References**

132 Source: [Article Notebook](#)